

analytic Continuation of Quantum Monte Carlo Data: Optimal Stochastic Regularization Approach

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A new algorithm for analytic continuation of quantum Monte Carlo (QMC) data from the Matsubara domain to real frequencies is proposed. Unlike the widely used maximum-entropy (MaxEnt) procedure, our method is linear with respect to the input data and can therefore be applied to off-diagonal components of Green's function, or to the self-energy function. The latter possibility is used to analyse QMC result for the half-filled Hubbard model on the Bethe lattice. Our method resolves the shoulders near the Hubbard band onsets, whereas the MaxEnt estimation does not.

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I. INTRODUCTION

Modern theoretical physics analysis of strongly correlated systems deals with a wide range of numerical methods, because no serious progress has yet been made in formulating a regular analytic description. In particular, progress has been achieved in Dynamical Mean Field Theory (DMFT)^{1,2}, as well as in its extensions and generalizations³. In the DMFT approach strongly-correlated systems are reduced to an effective impurity problem. Virtually, a single atom or small cluster is removed from the lattice but placed into a Gaussian bath defined in a self-consistent way. DMFT requires a so-called solver algorithm, which is intended to give an approximate evaluation of Green's functions for an effective impurity model. For the most cases, the Quantum Monte Carlo (QMC) class of solvers is used^{4,5}. These algorithms allow the calculation of electronic Green's functions for many models lying far beyond the regime where perturbation theory is valid. It is important to note that the output of QMC calculation belongs to the imaginary-time domain. This information is enough to evaluate DMFT loops, since DMFT equations are written in terms of fermionic Matsubara frequencies $\omega_n = (2n + 1)\pi/\beta$, where β is the inverse temperature.

On the other hand, experimental data is, of course, obtained in the real-time or real-frequency domain. Consequently, it is evidently quite a difficult problem to extract physical information from a numerical data set, because analytic continuation is needed.

In the canonical problem one has to obtain the spectral density function $A(\omega)$ from a noisy set of values for thermal Green's function $\mathcal{G}(\tau)$ or its Fourier transform $\mathcal{G}(i\omega_n) = \int_0^\beta d\tau e^{-i\omega_n\tau} \mathcal{G}(\tau)$, produced in a QMC simulation. The spectral density is proportional to imaginary part of retarded Green's function, from the definition:

$$A(\omega) = -\frac{1}{\pi} \text{Im} G^R(\omega) \quad (1)$$

Because of the analyticity of the retarded Green's function in the upper complex plane of frequency the follow-

ing is true:

$$G^R(\omega) = -\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Im} G^R(\omega')}{\omega - \omega' + i0} d\omega' = \int_{-\infty}^{+\infty} \frac{A(\omega')}{\omega - \omega' + i0} d\omega' \quad (2)$$

Substituting $\omega = i\omega_n$ one can derive the integral equation

$$\mathcal{G}(\tau) = \int_{-\infty}^{+\infty} d\omega \frac{e^{-\tau\omega}}{1 + e^{-\beta\omega}} A(\omega) \quad (3)$$

which is a particular formulation of the analytic continuation problem. The kernel of this integral equation is exponentially small at large positive and negative frequencies, so tiny variations in $\mathcal{G}(\tau)$ may correspond to a very strong change of the spectrum at those frequencies. Uncertainty in $\mathcal{G}(\tau)$ is unavoidable due to the stochastic nature of QMC algorithms, so the problem of numerical analytic continuation is extremely ill-posed, similarly to a numerical inversion of a Laplace transform.

The earliest attempts to solve the problem were based on Pade approximation method⁶. For a lot of cases, modifications of the standard least squares procedure has been proposed^{7,8}. Currently the most common practice is to use the Maximum Entropy algorithm for the analytic continuation problem⁹. It's based on Bayesian inference concept and essentially uses *a priori* knowledge about the properties of the spectral function, its positivity and sum rules. In other words, the MaxEnt algorithm is essentially a *nonlinear* formulation. Existing realizations of MaxEnt do not allow the analytic continuation of functions, whose norm is not a known constant (self-energy, for instance), or do not have a definite sign (for example, off-diagonal components of Green's function).

The aim of this paper is to introduce a new analytic continuation algorithm, which is linear with respect to input data and strong enough to be considered as an alternative for the MaxEnt method. Section II of the paper is devoted to the general idea behind the method without giving details of a particular realization. It explains optimal regularization principle, which is built on top

of Tikhonov regularization ansatz. Some more specific realization details are described in sections III and IV. They, in principle, may be revised and adjusted to a certain extent for specific problem. In Section V we present practical results of analytic continuation for the Hubbard model on the Bethe lattice, which is then compared with corresponding results from the MaxEnt algorithm. In Section VI we conclude the paper.

II. THE OPTIMAL REGULARIZATION MATRIX

Mathematically speaking, analytic continuation requires a solution of a linear integral equation for unknown function $F(\omega)$

$$\hat{M}F(\omega) = F(i\omega) \quad (4)$$

using certain *a priori* information. Here \hat{M} is the ill-posed linear operator which analytically continues from the real to the imaginary axis, and function $F(i\omega)$ is approximately known from a QMC simulation.

If we have introduced certain basis of orthogonal functions to represent $F(\omega)$ and $F(i\omega)$, the above integral equation becomes a set of linear algebraic equations

$$\hat{M}x = y, \quad (5)$$

where M is badly conditioned matrix, and the right hand part y is subject to some level of inaccuracy. Formally, the rank of the set is infinite. One would expect that for a properly chosen basis the effective reduction to a finite set is possible. Such a basis, suitable for the analytic-continuation problem is introduced in Section III.

The starting point of the proposed method is a Tikhonov regularization of the problem¹⁰. Let us search for a vector x , which minimizes the Tikhonov functional:

$$\mathcal{F}[x; \hat{R}] = \|\hat{M}x - y\|^2 + (x, \hat{R}x) \quad (6)$$

Here \hat{R} is a regularizing Hermitian matrix. Vector y is known approximately: $y = \bar{y} + \delta y$, where \bar{y} is the mean value of the vector y , and the deviation δy is a random quantity distributed with zero mean value and characterized by the covariation matrix \hat{K}_y , such that:

$$\overline{\delta y} = 0, \quad \hat{K}_y = \overline{\delta y \delta y^\dagger} \quad (7)$$

(hereafter the line over an expression denotes the QMC expectation).

Varying the functional $\mathcal{F}[x; \hat{R}]$ with respect to x , one obtains a condition for the vector x , which gives the minimum of the functional for given y and \hat{R} :

$$x = \hat{X} \hat{M}^\dagger y, \quad \text{where } \hat{X} \equiv (\hat{M}^\dagger \hat{M} + \hat{R})^{-1} \quad (8)$$

Assume that the vector \bar{x} is an exact solution of the set of equations (5) with an exactly known right-hand

part: $\hat{M}\bar{x} = \bar{y}$. We average the mean square deviation of x from \bar{x} over all possible values of the random vector δy to obtain the following:

$$\overline{\|x - \bar{x}\|^2} = \text{Tr}\{\hat{X} \hat{A} \hat{X} - 2\hat{X} \hat{B}\} + \text{Tr}\{\bar{x} \bar{x}^\dagger\} \quad (9)$$

$$\hat{A} \equiv \hat{M}^\dagger \hat{M} \bar{x} \bar{x}^\dagger \hat{M}^\dagger \hat{M} + \hat{M}^\dagger \hat{K}_y \hat{M} \quad (10)$$

$$\hat{B} \equiv \hat{M}^\dagger \hat{M} \bar{x} \bar{x}^\dagger \quad (11)$$

It should be obvious, that a proper choice of regularizing matrix R is required to provide a satisfactory small value of $\overline{\|x - \bar{x}\|^2}$. On the other hand, a desired type of the behavior of a solution \bar{x} cannot be determined or even estimated from the results of QMC simulation alone. Construction of a regularizing algorithm presumes utilization of certain *a priori* information about the properties of the solution.

Very generally, the use of *a priori* information means making an assumption that the result \bar{x} is not arbitrary, but falls into certain classes of possible solutions. For example, one can suppose that the resulting function is smooth, not too large, etc. We denote by $\langle \dots \rangle$ the average over possible class of the solutions. It is reasonable to require that the regularizing functional R delivers the minimum of the deviation $\overline{\|x - \bar{x}\|^2}$ in the average over the set of possible solutions,

$$\overline{\|x - \bar{x}\|^2} = \text{Tr}(\hat{X} \langle \hat{A} \rangle \hat{X} - 2\hat{X} \langle \hat{B} \rangle) + \text{Tr}\langle \bar{x} \bar{x}^\dagger \rangle = \min_{\hat{R}} \quad (12)$$

The main idea of the proposed method is to solve this minimum problem with respect to R and then to obtain x from (8). A specific choice of the possible class of solutions is discussed in Section IV. However already at this point it is worth noting that we actually do not need a complete information about the possible solutions, but only the first and the second momenta of x , since only these quantities appear in (12) (recall expressions (10, 11) for A and B).

Solving (12) with respect to \hat{R} and taking into account the additional condition $\delta \hat{R} = \delta \hat{R}^\dagger$, one obtains an equation for the matrix \hat{X} (the trivial solution $\hat{X} = 0$ does not relate to the problem):

$$\langle \hat{A} \rangle \hat{X} + \hat{X} \langle \hat{A} \rangle = \langle \hat{B} \rangle + \langle \hat{B}^\dagger \rangle \quad (13)$$

In this way we formally found a system of $N(N+1)/2$ linear equations for all elements of the matrix \hat{X} (where N is the dimension of the square matrix $\langle \hat{B} \rangle$). However, there is a more efficient way to solve the obtained equation (13).

Let us denote eigenvalues of the matrix $\langle \hat{A} \rangle$ by λ_i and perform an unitary transformation to a primed basis, in which $\langle \hat{A} \rangle$ is diagonal. In this basis a solution of equation (13) can be expressed explicitly:

$$x'_{ij} = \frac{b'_{ij} + (b^*_{ji})'}{\lambda_i + \lambda_j} \quad 1 \leq i, j \leq N \quad (14)$$

Changing to the eigenbasis of the matrix $\langle \hat{A} \rangle$ allows us to organize the numerical solving of the system (13) in an efficient way. The search procedure for eigenvalues and eigenvectors of $\langle \hat{A} \rangle$ is quite stable because $\langle \hat{A} \rangle$ is Hermitian. The advantage of such an approach in comparison with the direct solving of (13) is that instead of solving a system of $N(N+1)/2$ equations ($\propto N^6$ operations) it is enough to diagonalize the $N \times N$ matrix $\langle \hat{A} \rangle$ ($\propto N^3$ operations).

We should note that, mathematically, formula (14) unambiguously gives finite expressions for all the elements of \hat{X} , since its denominator is positive. Indeed the matrix $\hat{M}^\dagger \hat{M}$ is nonnegative definite. Matrix $\langle \bar{x} \bar{x}^\dagger \rangle$ is a correlation matrix, which is also essentially positive definite. Finally, the matrix \hat{K}_y is also positive definite, if the vector y is defined with nonzero inaccuracy (all components having nonzero dispersion). In this way we ensure that the matrix $\langle \hat{A} \rangle$ is positively defined and therefore all its eigenvalues are positive.

On the other hand, the practical realization of the method faces certain difficulties, because the numerical solution suffers from round-off errors in our calculations. The singular value decomposition procedure does not help much. To get rid of these round-off errors, we have switched to performing the calculations with to arbitrary number of digits, using CLN library version 1.1.13¹¹.

III. CHOICE OF REPRESENTATION. CORRELATION MATRIX

Now we apply results of the previous Section directly to the analytic continuation of a function $F(\omega)$ from the imaginary axis to the real one, assuming $F(\omega)$ to be analytic in the upper plane. QMC simulation gives values of the function F at Matsubara frequencies $i\omega_k$ on the imaginary axis:

$$F_k = F(i\omega_k), \quad k = \overline{1, K} \quad (15)$$

Let ω_0 be a typical frequency scale of the problem. Let us introduce a conformal mapping of the upper frequency plane to a circle of a unitary radius with the center at zero point:

$$\omega \rightarrow z: \quad z = \frac{\omega - i\omega_0}{\omega + i\omega_0}, \quad \omega = i\omega_0 \frac{1+z}{1-z} \quad (16)$$

The mapping is illustrated by figure 1. In this case all imaginary frequencies are mapped to a segment $z \in [-1; 1]$; all real frequencies correspond to the circle with radius 1.

If F is analytic in the upper plane as a function of complex frequency, it has the same property in the unit circle in the z -plane and can be expanded in the Taylor series at point $z = 0$:

$$F(\omega(z)) = \sum_{n=0}^{\infty} f_n z^n, \quad f_n = \frac{1}{2\pi i} \oint_{|z|=1} \frac{F(\omega(z))}{z^{n+1}} dz \quad (17)$$

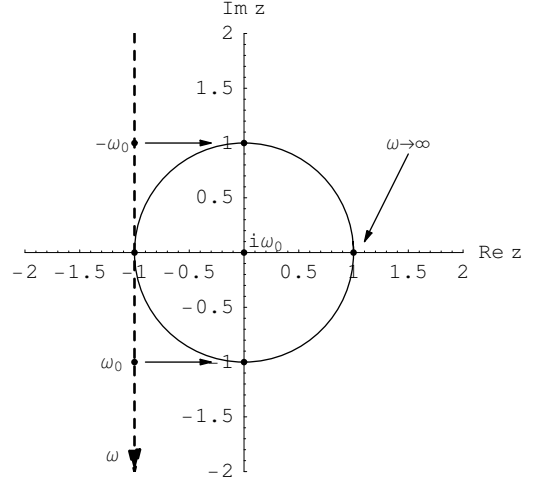


FIG. 1: Schematic view of the conformal mapping of upper frequency plane to a circle.

Assuming that the function $F(z)$ is smooth, we can then take into account a finite number of terms in this expansion. The proper number N of terms to be kept can be estimated from test runs of the program for a known function F . After the expansion coefficients f_n are determined, we can then sum up the series at any point of the circle $|z| = 1$ and thus restore values of $F(\omega)$ on the real axis.

The chosen representation \hat{M} entering equation (5) is then a $K \times N$ matrix with elements given by formula

$$M_{kn} = \left(\frac{\omega_k - \omega_0}{\omega_k + \omega_0} \right)^n \quad (18)$$

Using some *a priori* information about the expected solutions $F(\omega \in \mathbb{R})$, we can then choose a correlation matrix $\langle F(\omega) F^*(\omega') \rangle |_{\omega, \omega' \in \mathbb{R}}$. This correlation matrix also can be expanded into the double Taylor series at zero point, similarly to (17):

$$\langle F(\omega) F^*(\omega') \rangle |_{\omega, \omega' \in \mathbb{R}} \approx \sum_{n, n'=0}^{N-1} \langle f_n f_{n'}^* \rangle z^n (z')^{-n'} \quad (19)$$

$$\begin{aligned} \langle f_n f_{n'}^* \rangle &= \\ &= \frac{1}{(2\pi i)^2} \oint_{|z|=1} \oint_{|z'|=1} \langle F(\omega(z)) F^*(\omega(z')) \rangle z^{-(n+1)} z'^{-(n'-1)} dz dz' \end{aligned} \quad (20)$$

Practically, it was found that $N \approx 30 - 50$ terms is enough for the calculation. A value of ω_0 was not found to be really important; it is sufficient just to take ω_0 of the right order of magnitude.

IV. CORRELATION MATRIX OF LORENTZIAN PEAKS

The explicit form of the correlator $\langle F(\omega)F^*(\omega') \rangle$, leading to satisfactory results, can be obtained from the following procedure.

Let us assume that function F is a superposition of several Lorentzian peaks having the same width γ

$$F(\omega) = \sum_{j=1}^J \frac{Z_j}{\omega - \Omega_j + i\gamma} \quad (21)$$

The positions of the peaks Ω_j and their magnitudes Z_j are random quantities with known statistical properties

$$\langle F(\omega_1)F^*(\omega_2) \rangle = \sum_{j,j'=1}^J \left\langle \frac{Z_j}{\omega_1 - \Omega_j + i\gamma} \frac{Z_{j'}}{\omega_2 - \Omega_{j'} - i\gamma} \right\rangle_{Z,\Omega} \quad (22)$$

We assume that all Z_j are equally distributed and uncorrelated with each other, so that two model parameters $\langle Z^2 \rangle$ and $\langle Z \rangle$ completely determine the distribution of Z_j :

$$\langle F(\omega_1)F^*(\omega_2) \rangle = \langle Z^2 \rangle \sum_{j=1}^J \left\langle \frac{1}{\omega_1 - \Omega_j + i\gamma} \frac{1}{\omega_2 - \Omega_j - i\gamma} \right\rangle_{\Omega} + \langle Z \rangle^2 \sum_{j \neq j'}^J \left\langle \frac{1}{\omega_1 - \Omega_j + i\gamma} \frac{1}{\omega_2 - \Omega_{j'} - i\gamma} \right\rangle_{\Omega} \quad (23)$$

Finally we assume, that the values Ω_j are distributed independently with certain model distribution, for example the Lorentzian:

$$P(\Omega_j) = \frac{1}{\pi\Omega_M} \frac{1}{1 + (\Omega_j/\Omega_M)^2} \quad (24)$$

where Ω_M is the scale of the spectrum. For example, half of the Hubbard U is a good guess for this quantity in Hubbard-like models.

Combination of formulas (20) and (23) yields a result suitable for a practical calculations:

$$\begin{aligned} \langle f_n f_{n'}^* \rangle = & J \langle Z^2 \rangle \int_{-\infty}^{+\infty} P(\Omega) I(n, \gamma, \Omega) I^*(n', \gamma, \Omega) d\Omega + \\ & + J(J-1) \langle Z \rangle^2 \int_{-\infty}^{+\infty} P(\Omega_1) I(n, \gamma, \Omega_1) d\Omega_1 \int_{-\infty}^{+\infty} P(\Omega_2) I(n', \gamma, \Omega_2) d\Omega_2 \end{aligned} \quad (25)$$

$$I(n, \gamma, \Omega) \equiv \begin{cases} \frac{1}{i\gamma - \Omega + i\omega_0}, & n = 0 \\ -2i\omega_0 \frac{(i\gamma - \Omega - i\omega_0)^{n-1}}{(i\gamma - \Omega + i\omega_0)^{n+1}}, & n \neq 0 \end{cases}$$

Although these integrals could be calculated analytically for a particular Lorentzian form of $P(\Omega)$, the answer is very complicated and has significant computational complexity. It is therefore much more practical to perform an integration numerically for every pair of n and n' .

V. MOTT TRANSITION AT BETHE LATTICE: PRACTICAL CALCULATION OF DOS

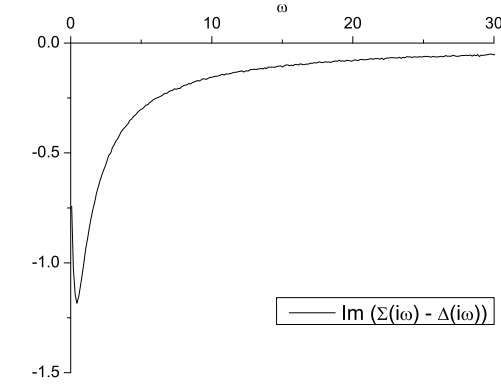
To illustrate the potential of the method, we reconstruct the density of states for the half-filled single-band Hubbard model defined on the Bethe lattice. Near-neighbor hopping constant for the model was equal to 0.5, and the Hubbard U ranged from 1.0 to 3.0. Inverse temperature in the simulations was $\beta = 50$. The Mott transition was observed between $U = 2.4$ and $U = 2.5$. Data for $\mathcal{G}(\tau)$ and $\mathcal{G}(i\omega_n)$ was produced by the DMFT self-consistent loop. The continuous-time QMC code¹²

was used as an impurity-problem solver. This version of the QMC solver is particularly suitable, because it can produce high-accuracy data for $\mathcal{G}(i\omega_n)$ directly in $i\omega$ -domain, up to quite high Matsubara frequencies.

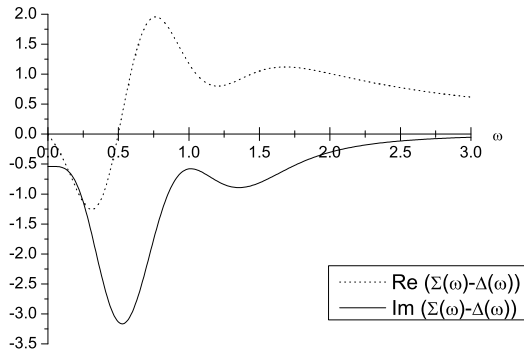
The regularization algorithm uses the model described in the previous section with the Gaussian distribution of Ω_j . An important peculiarity of the approach is that we work not with the Green's function, but with the quantity $\Sigma - \Delta$, defined by the relation

$$\mathcal{G}(i\omega_n) = \frac{1}{i\omega_n + \Delta(i\omega_n) - \Sigma(i\omega_n)} \quad (26)$$

Practically such a method has an advantage over the direct continuation of $\mathcal{G}(i\omega_n)$, because $\Sigma - \Delta$ does not have trivial $1/(i\omega)$ asymptotics. Therefore, a smaller number of z -harmonics is required for an adequate representation of this function. This also provides us with a physically important property $\int_{-\infty}^{\infty} A(\omega) d\omega = 1$, assuming that $\Delta - \Sigma$ remains finite as $\omega \rightarrow \infty$. Figure 2 illustrates the method, and Figure 3 shows the results for several values of U corresponding to metallic behavior. Unfortunately, the procedure works well only for the metal



(a)



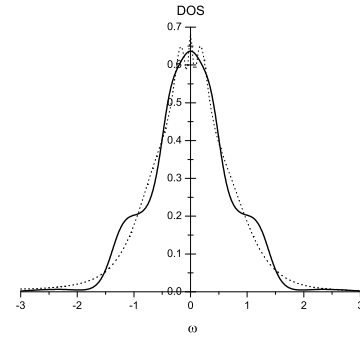
(b)

FIG. 2: (a) Input data for $\Sigma(i\omega_n) - \Delta(i\omega_n)$ at $U = 2.3$. (b) Reconstructed real and imaginary parts of $\Sigma(\omega) - \Delta(\omega)$. 300 Matsubara frequencies were used, with an estimated error bar in $\Sigma - \Delta$ is about 10^{-2} , the noise at different Matsubara frequencies was assumed to be uncorrelated. In the regularization procedure, the eigenvalues of 40×40 matrix have been obtained, using an accuracy to 80 decimal digits.

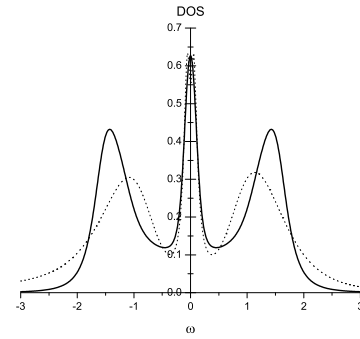
phase, because the insulator gap in DOS requires an infinite $\Sigma - \Delta$, which is clearly an impossible task for the continuation procedure.

For comparison, we present the result of MaxEnt calculation for the same QMC data. We have used a relatively simple MaxEnt program¹³. This code does not diagonalize the covariance matrix and uses a full search algorithm.

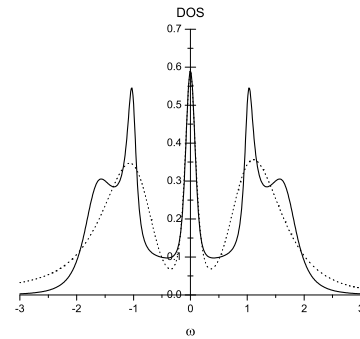
As can be seen from Figure 3, our procedure produces the data with much more details. Firstly, in all graphs the DOS decreases more rapidly at large energies. This is quite physical, one would expect that energy bands should be quite well confined. Secondly, in our case the shape of the dips at small energy in Figure 3 b,c is more similar to a “pre-formed” insulator gap. Finally, we were able to resolve very pronounced DOS shoulders near the onsets of the Hubbard bands. This agrees



(a)



(b)



(c)

FIG. 3: Reconstructed densities of states for $U = 1.0$, $U = 2.2$ and $U = 2.3$. Parameters of the regularization procedure are the same as in Fig.2. Results of the regularization are represented by solid lines. MaxEnt predictions are shown with dots.

well with the predictions of dynamical density-matrix renormalization-group theory¹⁴.

Of course, it should be noted that the particular appearance of the resulting graphs depends on a choice of *a priori* parameters Ω_M and γ . However, all qualitative peculiarities discussed in the previous paragraph are found to be quite robust against the variation of Ω_M and γ in a reasonable interval (approximately, from 0.1 to

2). Values of ω_0 , $\langle Z \rangle^2$ and $\langle Z^2 \rangle$ do not affect the result considerably, and so we put these quantities to 1 in the calculations.

VI. DISCUSSION AND CONCLUSIONS

To conclude, we developed a new regularization approach for the analytic continuation of numerical data from imaginary to real axis. The method is the best possible regularization in sense of (12), so that we produce an optimal regularization matrix given a class of possible solutions and errorbar of the input data.

An important property of the optimal regularization approach is its linearity with respect to the input data. This makes possible the continuation of the self-energy

and off-diagonal Green's function components. In principle, we could follow MaxEnt paradigm and put additional constraints like the requirement $A(\omega) \geq 0$. However this would make our scheme nonlinear and seriously reduce its flexibility. There is also negative consequences of the linearity of our approach: unphysical regions of negative DOS can occur for certain input data. It should also be noted that, accordingly to our observations, our method requires higher accuracy and larger number of Matsubara frequencies. In this case, our scheme has an advantage, as it is illustrated by the practical calculation for the Mott transition.

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¹¹ CLN library is distributed under GNU license. The current version is available at <http://www.ginac.de/CLN/>.

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